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The Extraction of Laminar Flow from Certain Brownian Motions

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Abstract—Using the concept of average velocity, we show that laminar flow can be extracted from Brownian motion. The flows studied are those around a flat, two dimensional plate on the molecular level. Flows of both water vapor and air are simulated.

Keywords—Fluid flow, Laminar, Brownian, Water vapor, Air.

1. INTRODUCTION

In this paper, we will show how to extract laminar flows from a class of Brownian motions associated with the planar flow of molecules around a flat plate. Flows around plates in the large have been studied extensively by fluid dynamicists (see, e.g., [1]). The flow which we will explore is on the nano level.

2. MATHEMATICAL AND PHYSICAL PRELIMINARIES

Let us consider first an approximate Lennard-Jones potential for water vapor molecules, which we take to be

$$\phi\left(r_{ij}\right) = (1.9646)\, 10^{-13} \left[\frac{2.725^{12}}{r_{ij}^{12}} - \frac{2.725^{6}}{r_{ij}^{6}}\right] \text{erg} \left(\frac{\text{grcm}^2}{\text{sec}^2}\right) \tag{2.1}$$

in which r_{ij} is measured in angstroms (Å). The force $\vec{F}_{ij}$ exerted on P_i by P_j is then

$$\vec{F}_{ij} = (1.9646)\, 10^{-5} \left[\frac{12(2.725^{12})}{r_{ij}^{13}} - \frac{6(2.725^{6})}{r_{ij}^{7}}\right] \frac{\vec{r}_{ji}}{r_{ij}} \text{dynes} \left(\frac{\text{grcm}}{\text{sec}^2}\right). \tag{2.2}$$

From (2.2), it follows that the equilibrium distance between two molecules is 3.05Å.

Note immediately that there is no known potential for liquid water. The primary reason for this is that close liquid water molecules exhibit hydrogen bonding. Formula (2.1) is, in fact, the Lennard-Jones portion of formula of Rowlinson for water vapor [2].

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3. APPROXIMATE EQUATIONS OF MOTION FOR WATER VAPOR MOLECULES

From the discussion in Section 2, it follows that the equation of motion for a single water vapor molecule P_i acted on by a single water vapor molecule P_j, $i \neq j$, is

$$m_i \vec{a}_i = (1.9646)10^{-5} \left[\frac{12(2.725^{12})}{r_{ij}^{13}} - \frac{6(2.725^6)}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}}. \tag{3.1}$$

Since the mass of a water molecule is $(30.103)10^{-24}$ gr, equation (3.1) is equivalent to

$$\vec{a}_i = (160.33)10^{19} \left[\frac{818.90}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}} \left(\frac{\text{cm}}{\text{sec}^2} \right). \tag{3.2}$$

For computational convenience, we rewrite equation (3.2) in Å/(ps^2), to yield

$$\vec{a}_i = (160330.) \left[\frac{818.90}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}} \left(\frac{\text{Å}}{\text{ps}^2} \right). \tag{3.3}$$

On the molecular level, however, the effective force on P_i is local, that is it is determined only by close molecules, by which we will mean only those molecules within a distance D determined by

$$\frac{dF_{ij}}{dr_{ij}} = 0.$$

The solution to this equation yields $r_{ij} = 3.39$Å. Thus, for $r_{ij} \geq D = 3.39$Å we choose $\vec{F}_{ij} = \vec{0}$. Note that we could define D in terms of 2σ or 3σ, which is more customary. However, the neglected molecular attraction is relatively insignificant because repulsion dominates so forcefully in the problems to be considered.

From (3.3), then, the dynamical equation for water molecule P_i will be

$$\frac{d^2\vec{r}_i}{dt^2} = (160330.) \sum_{\substack{j \neq i \\ j}} \left[\frac{818.90}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}}; \qquad r_{ij} < D. \tag{3.4}$$

The equations of motion for a system of water vapor molecules are then

$$\frac{d^2\vec{r}_i}{dt^2} = (160330) \sum_{\substack{j \neq i \\ j}} \left[\frac{818.90}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}}; \qquad i = 1, 2, 3, \ldots, N; \quad r_{ij} < D. \tag{3.5}$$

Observe that on the molecular level gravity can be neglected since

$$980\,\text{cm/sec}^2 = (980)10^{-16}\,\text{Å/ps}^2.$$

Note also, that in simulating the motion of a system of molecules, nonlinear equations (3.5) forewarn us that we will probably have to solve large systems of nonlinear, second order, ordinary differential equations and that these will have to be solved numerically. The leap frog formulas will be used for this purpose [3].

4. PROBLEM FORMULATION

Unless otherwise specified, the following general problem will be studied.

We first generate 49756 water molecules using the following recursion formulas:

$$x(1) = y(1) = 0.0,$$
$$x(i+1) = x(i) + 3.05, \quad y(i+1) = 0.0, \qquad i = 1, 260,$$
$$x(262) = 1.525, \qquad y(262) = 2.64,$$
$$x(i+1) = x(i) + 3.05, \quad y(i+1) = 2.64, \qquad i = 262, 520,$$
$$x(i) = x(i-521), \quad y(i) = y(i-521) + 5.28, \qquad i = 522, 49756.$$

We would like to replace various molecules by a rigid plate which is at a 45° angle in the basin. To do this conveniently we first rotate the particles generated above 45° by the formulas:

$$x^*(i) = 0.965925826289068x(i) + 0.258819045102521y(i), \qquad i = 1, 49756,$$
$$y^*(i) = 0.965925826289068y(i) - 0.258819045102521x(i), \qquad i = 1, 49756.$$

Next, we decrease the number of molecules to 12420 by choosing from the above set only those which lie in the rectangle $129 \le x \le 529$, $0 \le y \le 250$. Finally we translate all these by

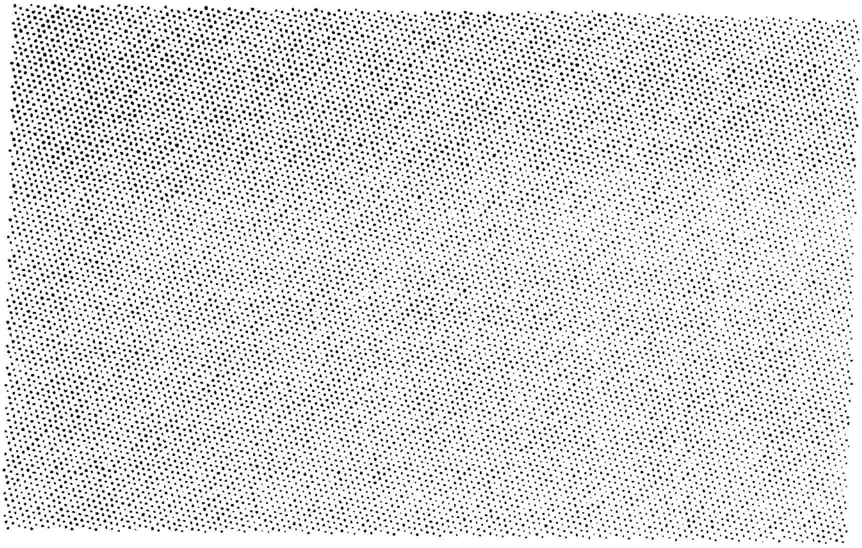

Figure 1. 12420 points.

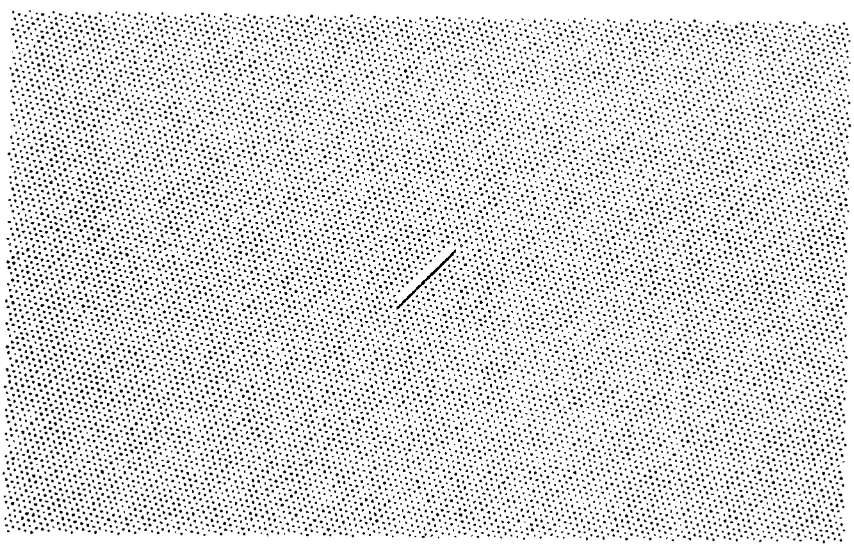

Figure 2. 12672 points.

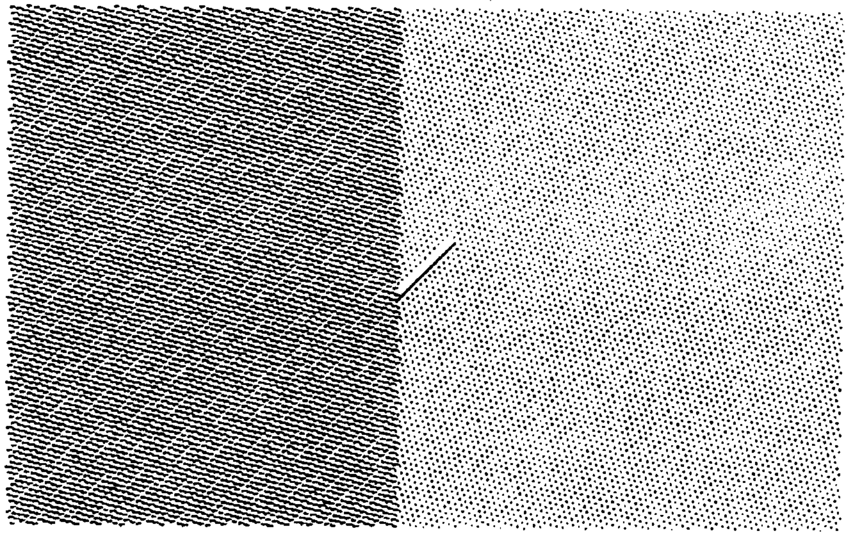

Figure 3. Initial velocities to left of the plate.

$x(i) = x^*(i) - 329$, so that the 12420 molecules lie in the rectangle $-200 \le x \le 200$, $0 \le y \le 250$. This result is shown in Figure 1. Next, we insert a 278 particle plate with a 45° slope between the two points $(-13.8673, 109.6126)$ and $(13.8327, 137.3127)$ and delete all molecules which are immediately adjacent to the plate and above it. This is shown in Figure 2, which has 12394 vapor molecules and 278 fixed plate particles.

We now have the basin with the desired plate and are ready to simulate flow around the plate. For this reason, we now assign to each molecule to the left of the plate a speed V in the x direction. Thus we now have the configuration shown in Figure 3. The top of Figure 3, whose equation is $y = 250$, and bottom, whose equation is $y = 0$, will be taken as fixed walls. The region to the right of the plate will be called the shadow region.

Our problem is to describe the resulting flow around the plate.

For time step Δt(ps), and $t_k = k\Delta t$, $k = 0, 1, 2, \dots$, two problems must be considered relative to the computations. The first problem is to prescribe a protocol when, computationally, a molecule has crossed a fixed wall into the exterior of the cavity. For each of the upper and lower walls, we will proceed as follows (no slip condition). The position will be reflected back symmetrically, relative to the wall, into the interior of the basin, the velocity component tangent to the wall will be set to zero and the velocity component perpendicular to the wall will be multiplied by -1. In addition if the molecule has crossed the plate, then it will be reflected back symmetrically and its x and y components of velocity will be replaced by its y and x components.

The second problem derives from the fact that an instantaneous velocity field for molecular motion is Brownian. In order to better interpret gross fluid motion, we will introduce average velocities as follows. For J a positive integer, let particle P_i be at $(x(i,k), y(i,k))$ at t_k and at $(x(i,k-J), y(i,k-J))$ at t_{k-J}. Then the average velocity $\vec{v}_{i,k,J}$ of P_i at t_k is defined by

$$\vec{v}_{i,k,J} = \left(\frac{x(i,k) - x(i,k-J)}{J\Delta t}, \frac{y(i,k) - y(i,k-J)}{J\Delta t} \right). \tag{4.1}$$

In the examples to be described, we will discuss results for various values of J.

5. EXAMPLES

EXAMPLE 1. For our first example let $V = 35$, $\Delta t = 4(10)^{-6}$, $J = 60000$. Then Figures 4–12 show the resulting laminar flow at the respected times $T = 0.36$, 0.60, 0.84, 1.08, 1.32, 1.56, 1.80, 2.04, 2.28. The most noticeable aspect of the flow is its movement below the plate and

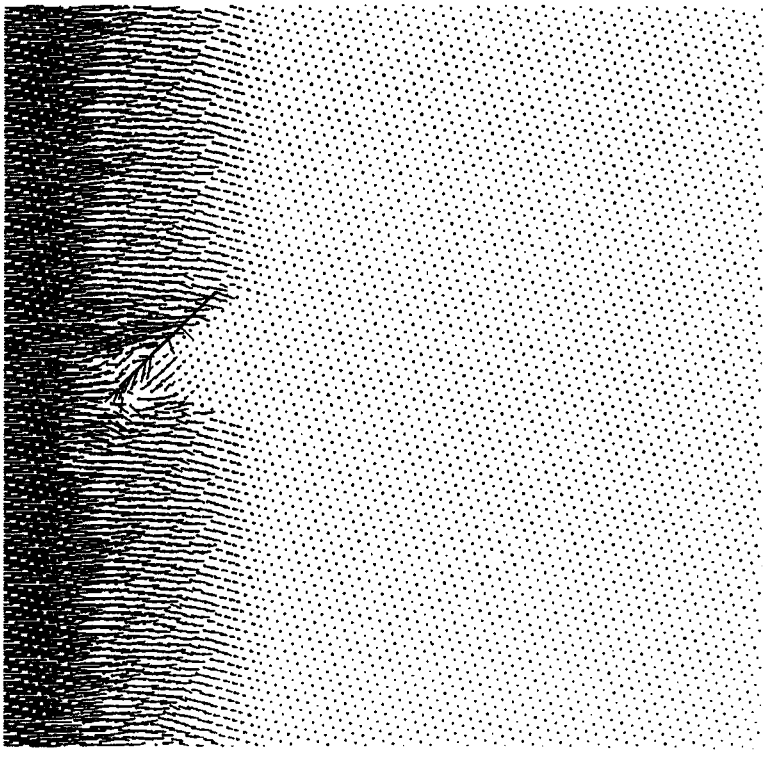

Figure 4. $V = 35$, $T = 0.36$.

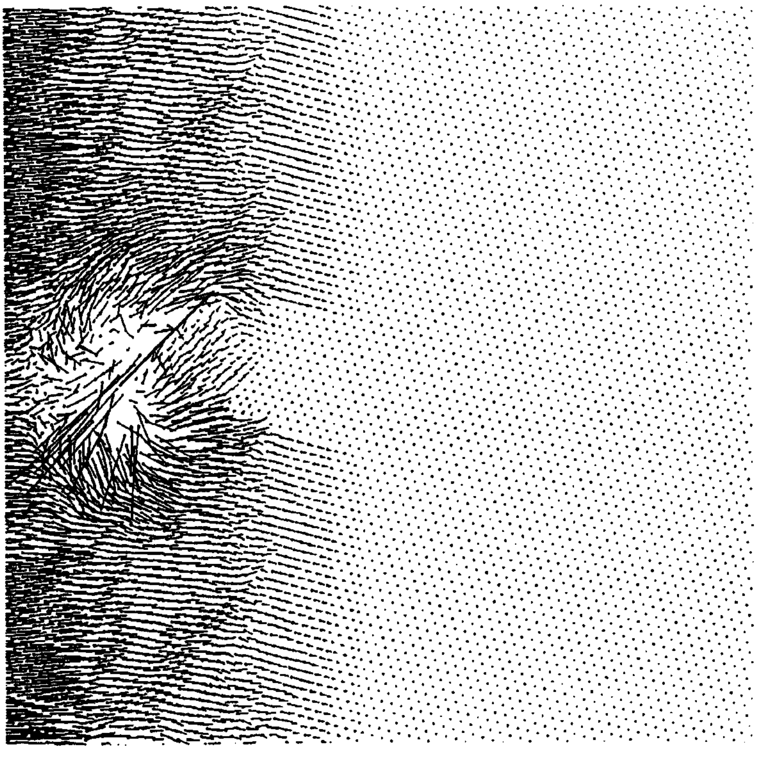

Figure 5. $V = 35$, $T = 0.60$.

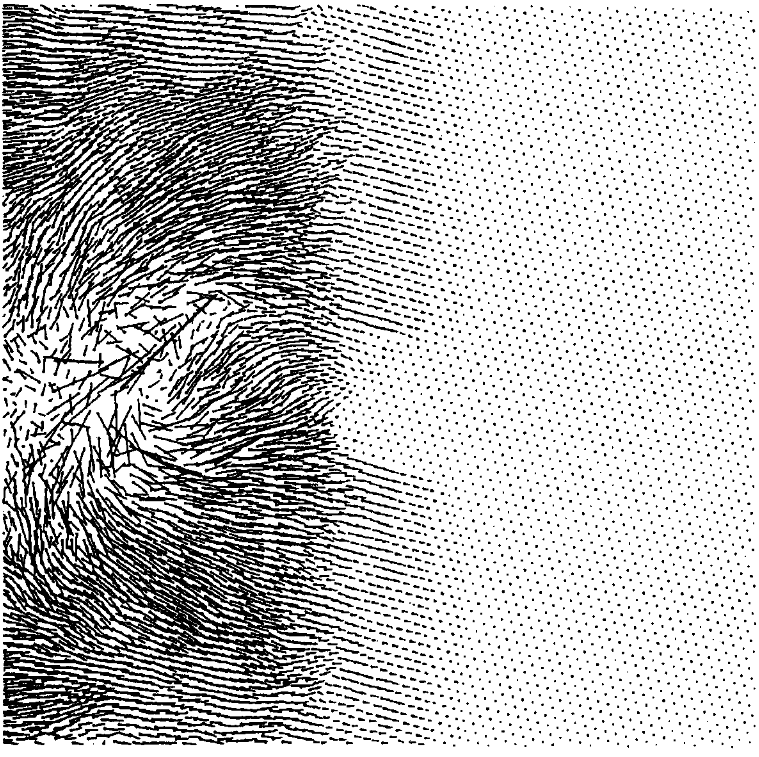

Figure 6. $V = 35$, $T = 0.84$.

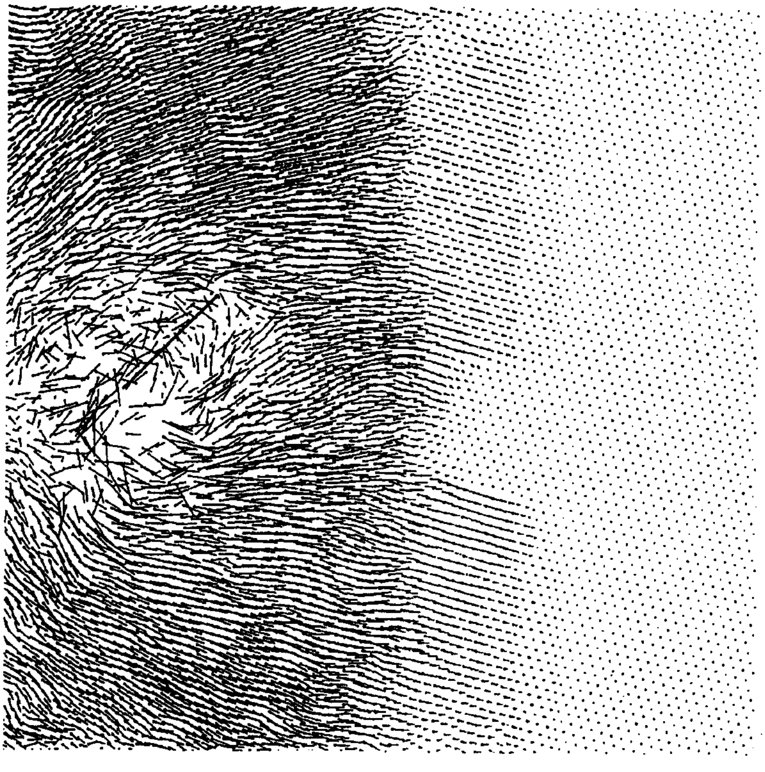

Figure 7. $V = 35$, $T = 1.08$.

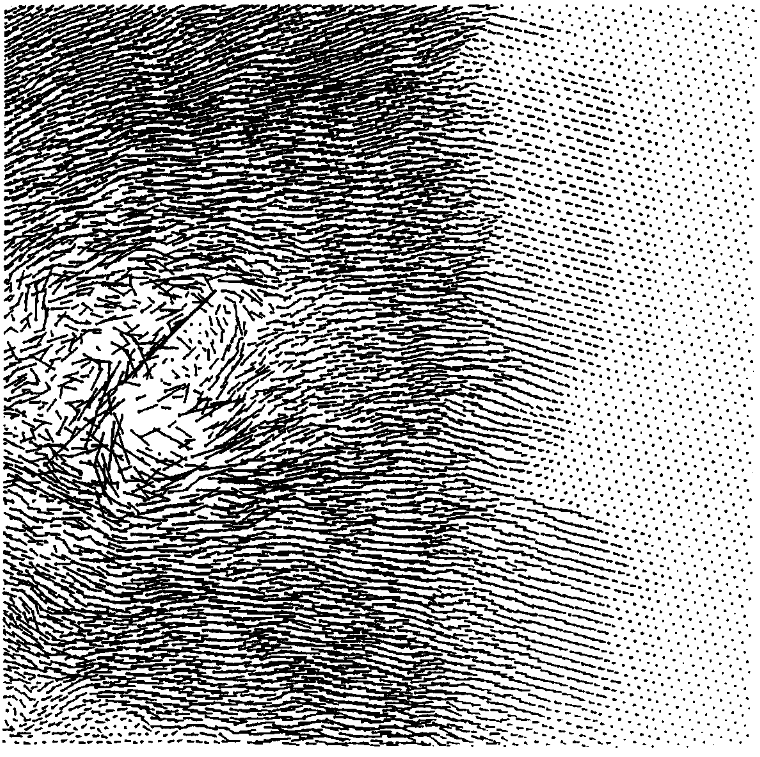

Figure 8. $V = 35$, $T = 1.32$.

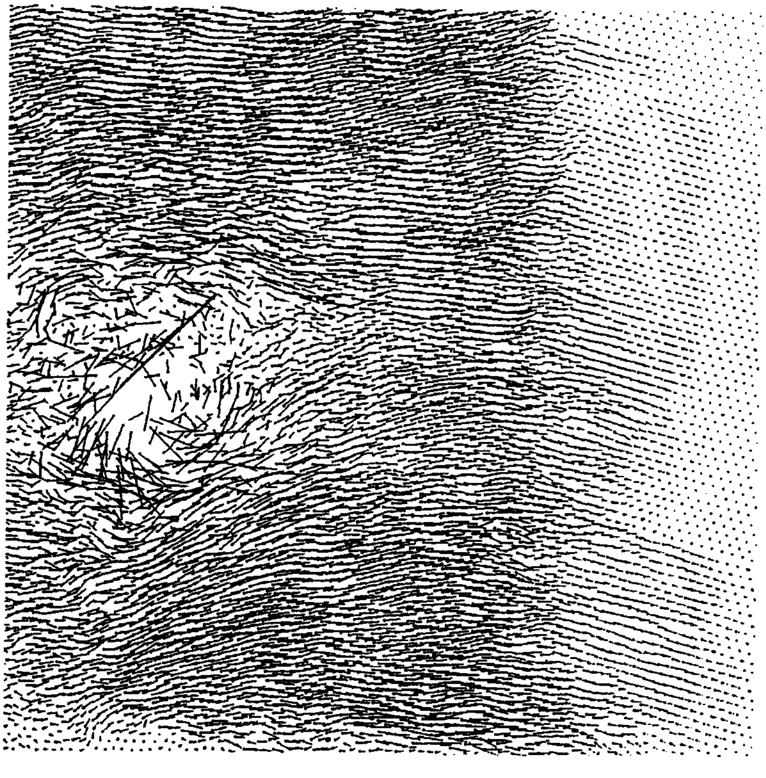

Figure 9. $V = 35$, $T = 1.56$.

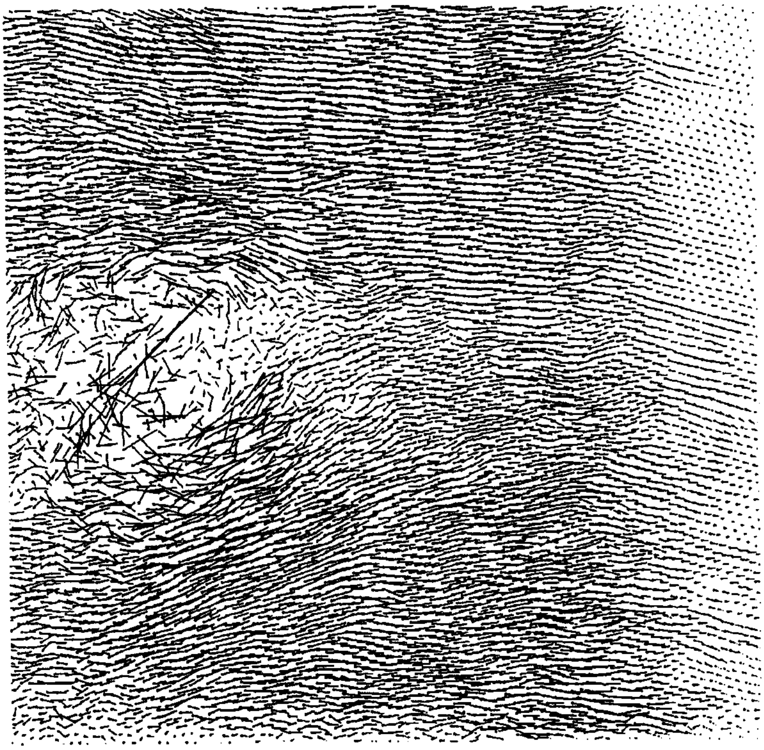

Figure 10. $V = 35$, $T = 1.80$.

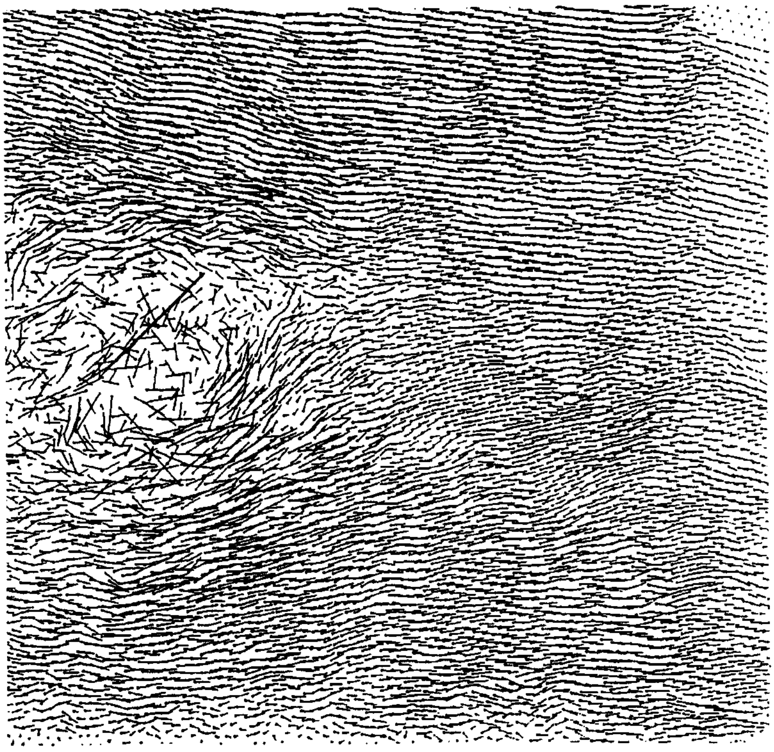

Figure 11. $V = 35$, $T = 2.04$.

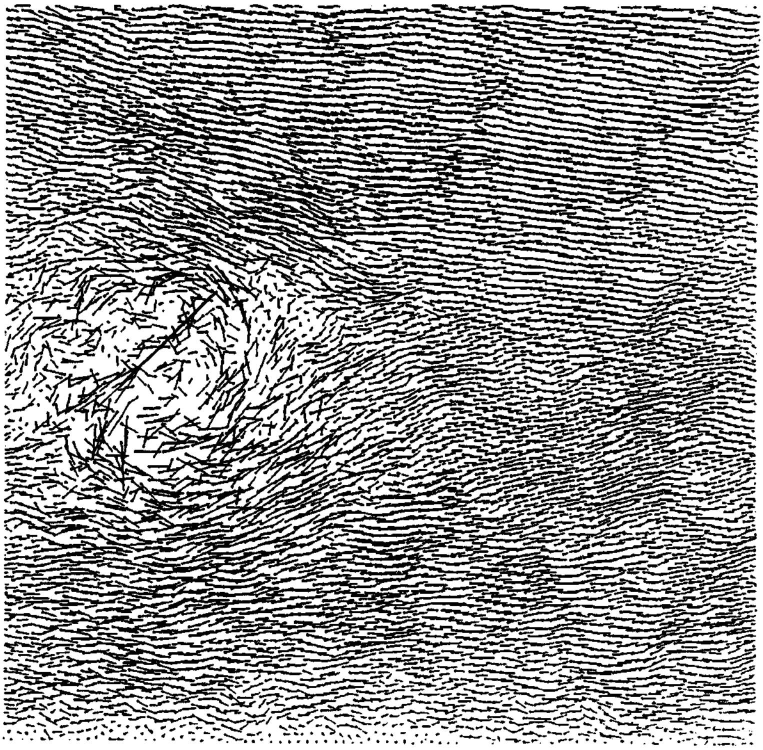

Figure 12. $V = 35$, $T = 2.28$.

then up into the shadow region. Figure 13 shows the instantaneous Brownian motion of the flow at $T = 1.32$ and should be compared with Figure 8. Similar results were obtained for $J = 30000, 90000$.

EXAMPLE 2. Example 1 was modified by setting $V = 20$, $\Delta t = 8(10)^{-6}$. The flow was entirely similar to that of Example 1 but developed more slowly. Figure 14 shows the flow at $T = 2.16$ and should be compared to the flows shown in Figures 7 and 8 at times $T = 1.08, 1.32$. The vectors in Figure 14 should be smaller than those in Figures 7 and 8, but have been rescaled for clarity.

EXAMPLE 3. Example 1 was modified by setting $V = 55$. The flow was entirely similar to that of Example 1, but developed more rapidly. Figure 15 shows the flow at $T = 1.84$ and should be compared with Figures 11 and 12.

EXAMPLE 4. Example 1 was modified by setting $V = 500$, $\Delta t = 4(10)^{-7}$, $J = 120000$. Figure 16 shows the flow at the early time $T = 0.284$. The flow is entirely similar to that in Example 1 but has developed more rapidly. It should be compared with Figure 10 at $T = 1.80$.

EXAMPLE 5. Example 1 was modified by setting $V = 6000$, $\Delta t = 4(10)^{-8}$, $J = 180000$. Figure 17 shows the flow at $4.8(10)^{-7}$. The flow now differs from all previous examples in that there is a strong current below the plate which crosses the usual laminar flow direction. Indeed, such a situation implies, in the large, the presence of turbulence [4]. Indeed, physically, a viewer does not see the velocity field in Figure 17. The viewer sees in the area below the plate [5] the rapid appearance and disappearance of small vortices. At $T = 4.8(10)^{-7}$, there are 12 such vortices in the range $-20 < x < 20$, $40 < y < 80$ and these are centered at

$$(-14.47, 44.25), (-15.53, 41.92), (-8.69, 49.93), (4.77, 46.52),$$
$$(14.31, 41.57), (-12.93, 57.97), (4.93, 54.35), (1.14, 58.19),$$
$$(5.89, 62.07), (-5.36, 76.55), (7.16, 67.10), (-6.13, 66.99).$$

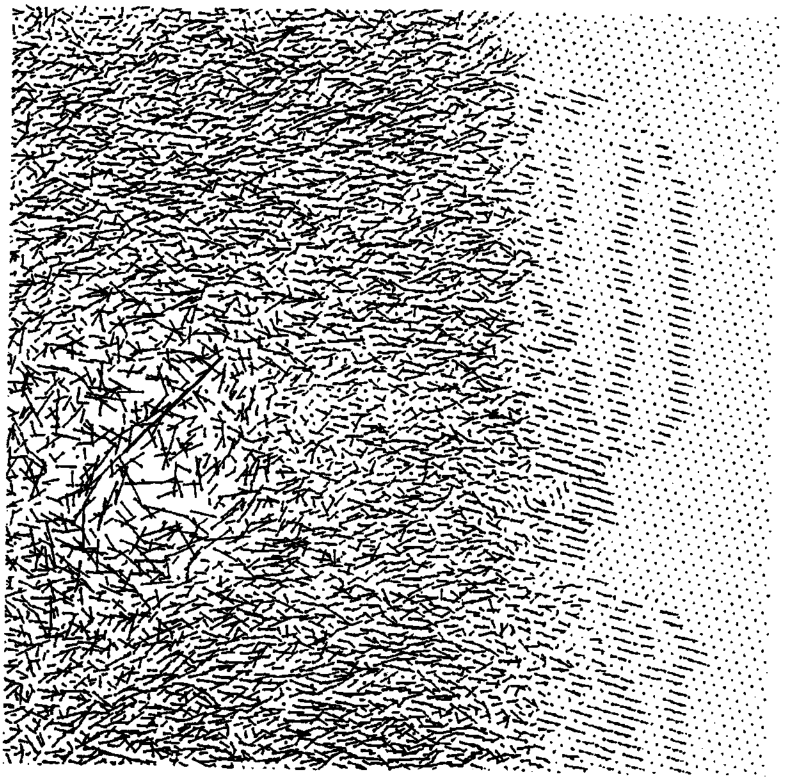

Figure 13. Brownian motion for $V = 35$, $T = 1.32$.

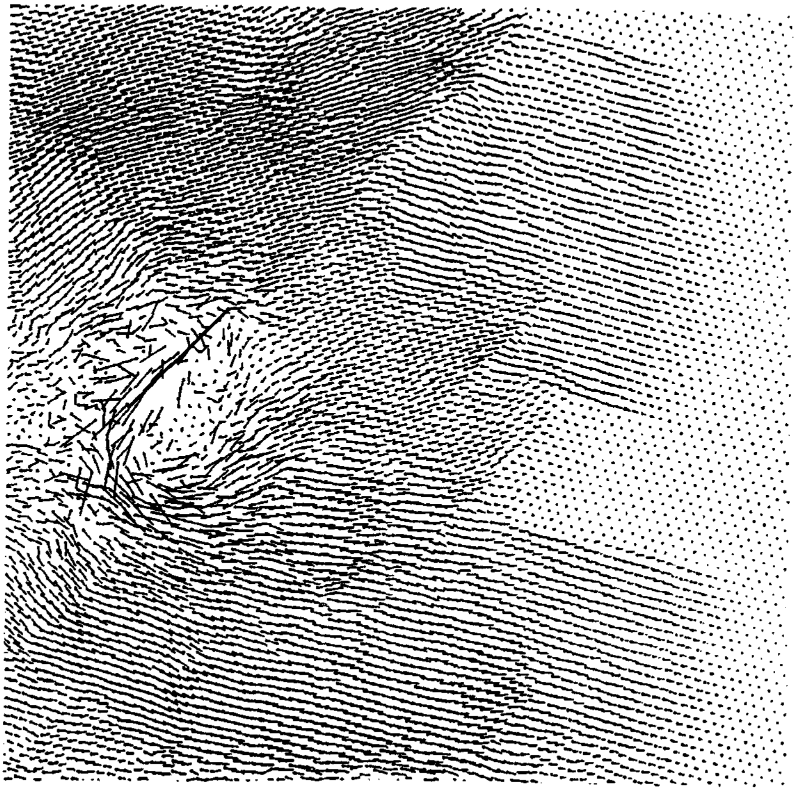

Figure 14. $V = 20$, $T = 2.16$.

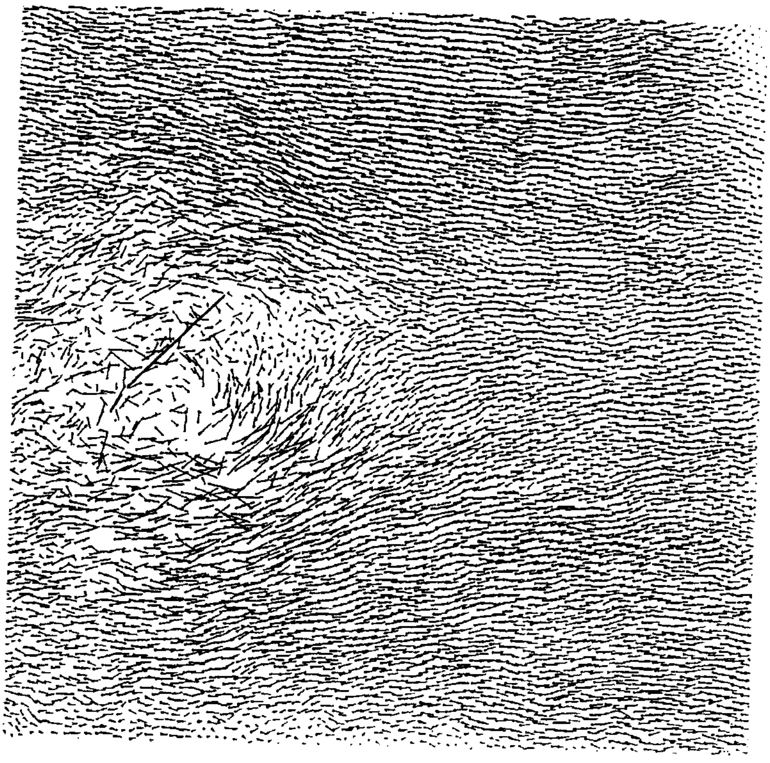

Figure 15. $V = 55$, $T = 1.84$.

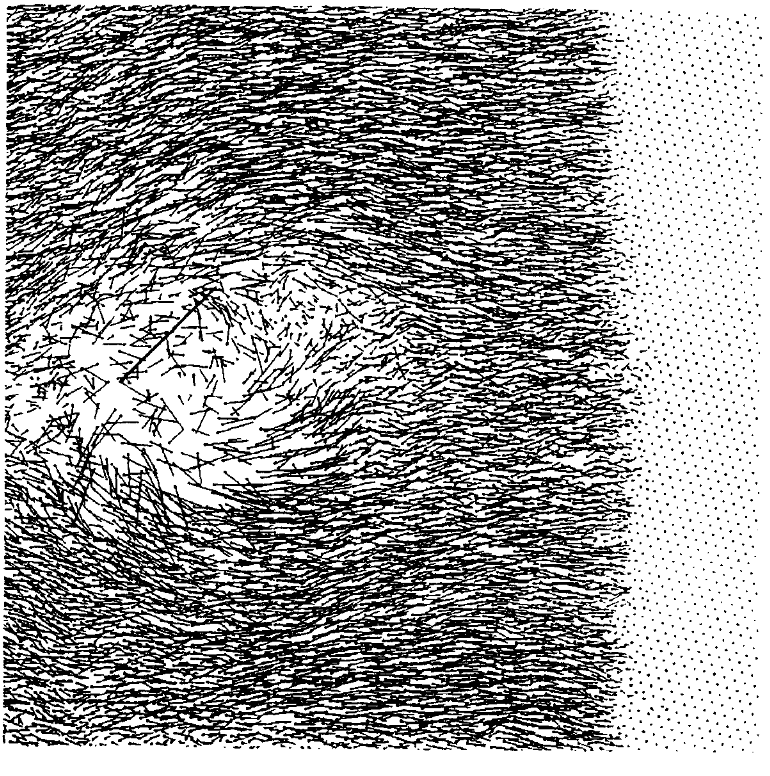

Figure 16. $V = 500$, $T = 0.284$, $J = 120000$.

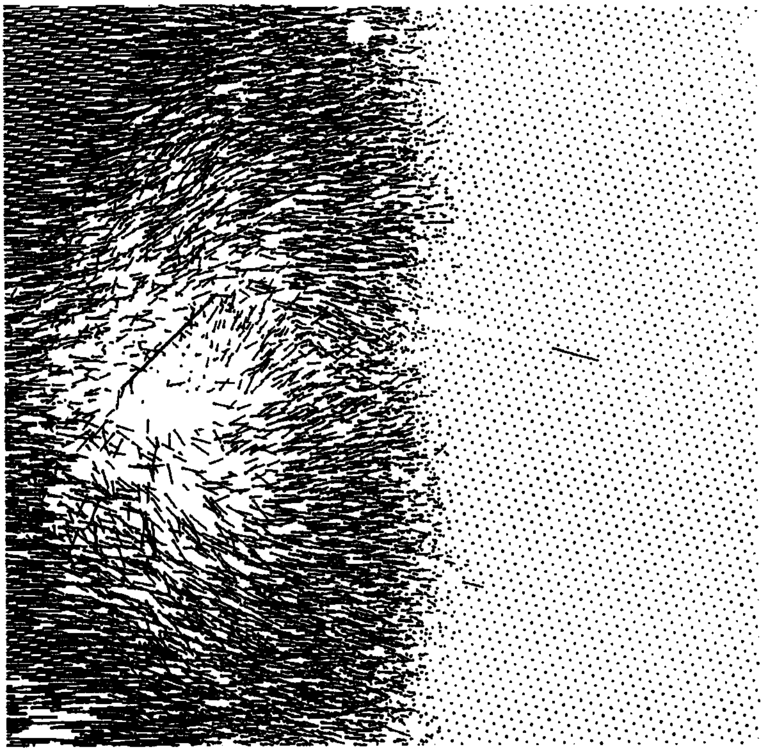

Figure 17. $V = 6000$, $T = 4.8(10)^{-7}$, $J = 180000$.

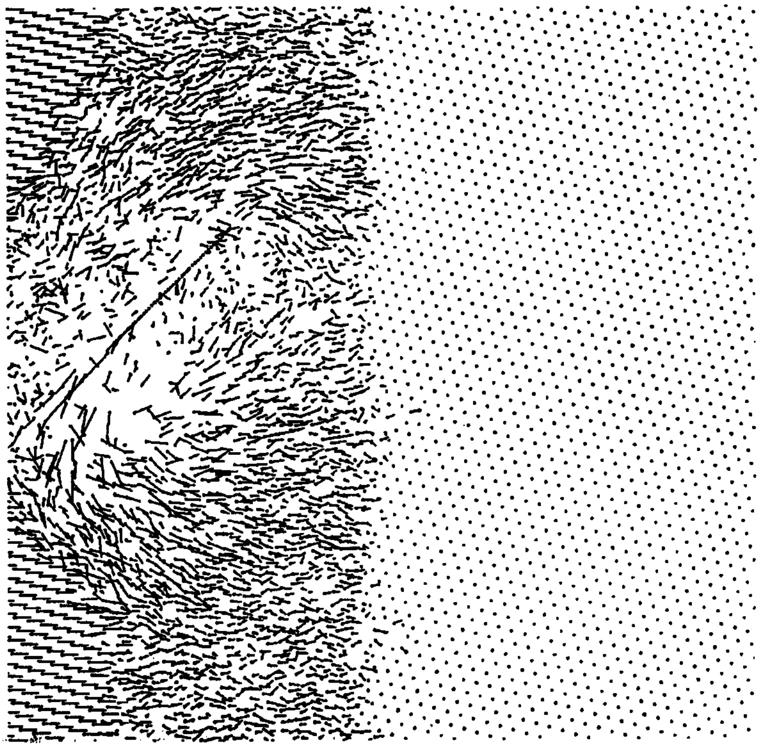

Figure 18. $V = 500$, $T = 0.159$, $J = 120000$.

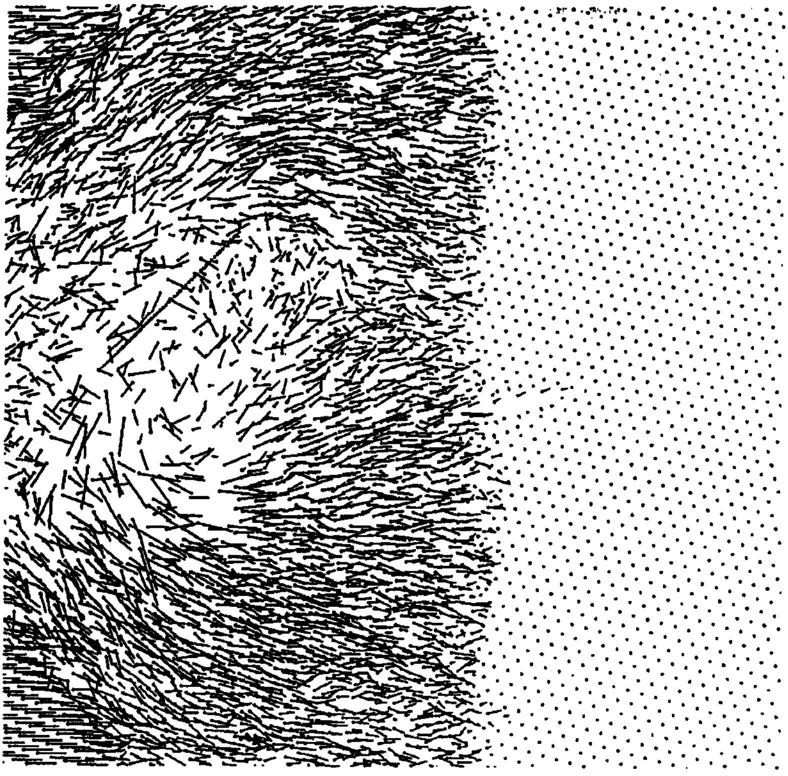

Figure 19. $V = 500$, $T = 0.223$, $J = 120000$.

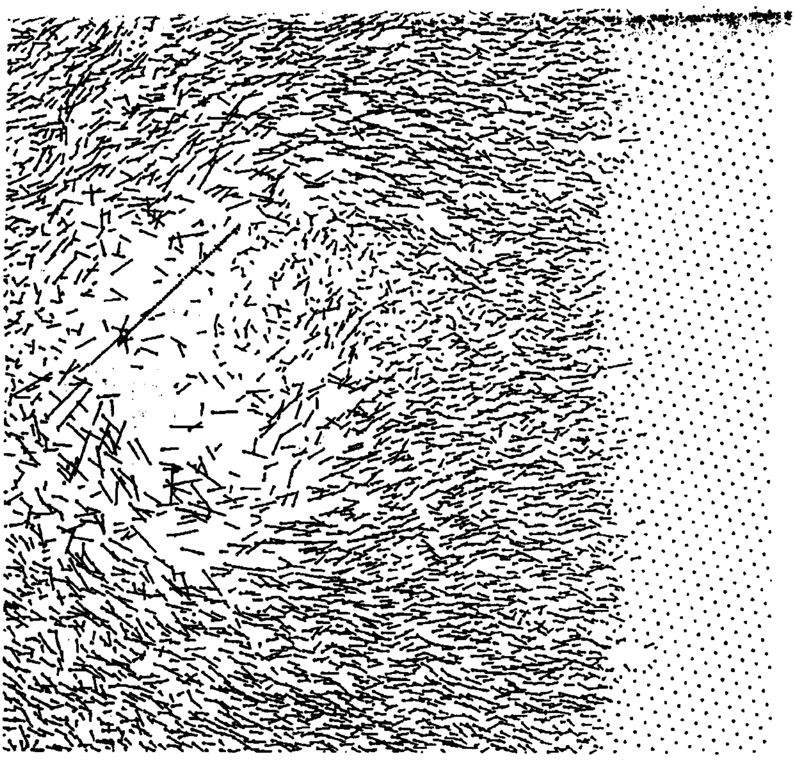

Figure 20. $V = 500$, $T = 0.294$, $J = 120000$.

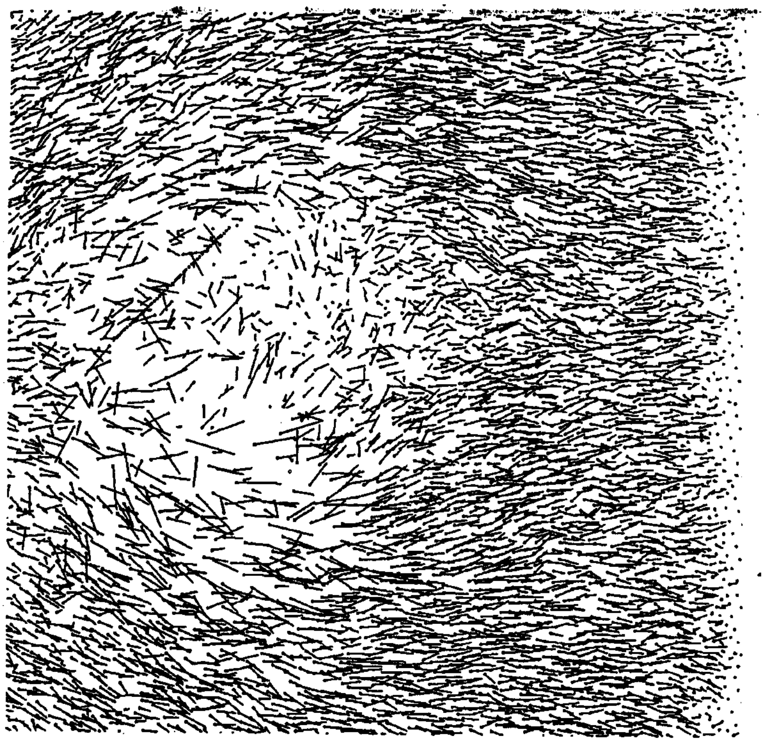

Figure 21. $V = 500$, $T = 0.366$, $J = 120000$.

At $T = 4.8(10)^{-7}$ there are 11 vortices which are centered at

$$(-17.98, 41.21), (3.07, 43.28), (11.36, 41.98), (12.25, 50.78),$$
$$(1.76, 49.76), (9.06, 47.83), (-12.90, 58.84), (14.03, 56.63),$$
$$(13.03, 53.58), (-19.41, 70.77), (0.91, 46.48).$$

Thus, in only $4(10)^{-8}$ sec, the vortices have changed in both number and in position. Note also that completely analogous results followed for $J = 240000$, $J = 210000$, $J = 150000$, $J = 120000$.

EXAMPLE 6. Example 5 was modified by setting $V = 3000$. The results were similar to those of Example 5 but were not as sharply defined.

6. REMARKS

Examples entirely analogous to those in Section 5 were repeated, but for air rather than for water vapor. The results were similar, but not identical . Figures 18–21 show the results for $V = 500$, $J = 120000$, at the respective times $T = 0.159, 0.223, 0.294, 0.366$. Typically, the flow for air is more dilute immediately behind the plate than for water vapor. Figure 20 should be compared with Figure 16.

REFERENCES

1. M. Van Dyke, *An Album of Fluid Motion*, pp. 88–103, Parabolic, Stanford, (1982).
2. J.O. Hirschfelder, C.F. Curtiss and R.B. Bird, J. Wiley & Sons, 1033–1034, (1967).
3. D. Greenspan, *Particle Modeling*, Birkhauser, Boston, MA, (1998).
4. H. Schlichting, *Boundary Layer Theory*, Fourth Edition, McGraw-Hill, New York, (1960).
5. D. Greenspan, Molecular cavity flow, *Fluid Dyn. Res.* **25**, 37–56, (1999).